Data Evaluation Record on the bioaccumulation of saflufenacil [BAS 800 H] in fish

PMRA Document Number 1547156 EPA MRID Number 47127909
PMRA Submission Number 2008-0431

Data Requirement: PMRA Data Code: 9.5.6
EPA DP Barcode: 349858
OECD Data Point: IIA 6.2.5
EPA Guideline: 850.1730

Test material:

Common name:	Saflufenacil.
Chemical name:	
IUPAC name:	N′-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide. N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.
CAS name:	2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.
CAS No:	372137-35-4.
Synonyms:	BAS 800 H, CL No. 433379, 4054449, AC 433,379.
SMILES string:	N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

EPA Reviewer: Greg Orrick
USEPA
Signature: Greg Orrick
Date: June 8, 2009

PMRA Reviewer: Ann Lee (1639)
HC-PMRA-EAD
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Date: 2008 November 28

APVMA Reviewer: Farzad Jahromi
APVMA
Signature:
Date:

Company Code: BAZ
Active Code: SFF
Use Site Category: 13 and 14
EPA PC Code: 118203

CITATION: Hafemann, C. 2007. Bioaccumulation and metabolism of BAS 800 H in bluegill sunfish (*Lepomis macrochirus*). Unpublished study performed by BASF Aktiengesellschaft, Limburgerhof, Germany; and sponsored and submitted by BASF Corporation, Research Triangle Park, North Carolina. Report Number: 132626. BASF Registration Document Number: 2007/1056242. Study initiated March 15, 2007 (in life phase); completion date July 18, 2007 (analytical phase; p. 9; Appendix 1, p. 30). Final report issued November 15, 2007. (MRID 47127909. PMRA Number: 1547156.)

Data Evaluation Record on the bioaccumulation of saflufenacil [BAS 800 H] in fish

PMRA Submission Number {.....} EPA MRID Number 47127909

Data Requirement: PMRA Data Code:
EPA DP Barcode: D349858
OECD Data Point:
EPA Guideline: 850.1730
OPPTS Guideline: 850.1730

Test material:

Common name:	Saflufenacil.
Chemical name:	
IUPAC name:	N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide. N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.
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Primary Reviewer: Amy Barnes
Cambridge Environmental
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Company Code:
Active Code:
Use Site Category:
EPA PC Code: 118203

CITATION: Hafemann, C. 2007. Bioaccumulation and metabolism of BAS 800 H in bluegill sunfish (*Lepomis macrochirus*). Unpublished study performed by BASF Aktiengesellschaft, Limburgerhof, Germany; and sponsored and submitted by BASF Corporation, Research Triangle

In fish exposed at the **low dose (1.0 µg/L)**, [^{14}C]saflufenacil residues reached steady state within 14 days of exposure, with mean whole body concentrations of 4.81 µg/kg, according to the study author. Maximum mean [^{14}C]saflufenacil residues were 4.81 µg/kg (exposure day 14) in whole fish, 0.35 µg/kg (exposure day 21) in edible tissue, and 6.09 µg/kg (exposure day 14) in inedible tissue. The study author calculated a mean BCF value of 3.91 for whole fish. Reviewer-calculated maximum mean BCF values were **4.63** for whole fish (14 days exposure), **0.33** for edible tissue (21 days exposure), and **5.86** for inedible tissue (14 days exposure). In edible and inedible tissue samples, [^{14}C]saflufenacil residues ranged from 0-0.35 µg/kg and 4.91-5.89 µg/kg at 21-28 days, respectively. The uptake rate constant (K_1) and kinetic bioconcentration factor (BCF_K) for whole fish were not reported. Tissue samples were not analyzed for [^{14}C]saflufenacil or its transformation products.

Following 16 days of depuration, [^{14}C]saflufenacil residues in the whole fish decreased by a mean of 70.5% at 16 days of depuration. The depuration half-life of the residues in the whole fish was not reported. The depuration rate constant (K_2) was not reported.

In fish exposed at the **high dose (10 µg/L)**, [^{14}C]saflufenacil residues reached steady state within 14 days of exposure, with mean whole body concentrations of 4.39 µg/kg, according to the study author. Maximum mean [^{14}C]saflufenacil residues were 17.87 µg/kg in whole fish (exposure day 24), 0.35 µg/kg in edible tissue (exposure day 21), and 23.68 µg/kg in inedible tissue (exposure day 24). The study author calculated a mean BCF value of 1.0 for whole fish. Reviewer-calculated maximum mean BCF values were **1.57** for whole fish (24 days exposure), **0.03** for edible tissue (21 days exposure), and **2.08** for inedible tissue (24 days exposure). In edible and inedible tissue samples, [^{14}C]saflufenacil residues ranged from 0.00-0.35 µg/kg and 6.30-23.68 µg/kg at 21-28 days, respectively. The uptake rate constant (K_1) and kinetic bioconcentration factor (BCF_K) for whole fish were not reported. Tissue samples were not analyzed for [^{14}C]saflufenacil or its transformation products.

Following 16 days of depuration, [^{14}C]saflufenacil residues in the whole fish increased by a mean of 2.3% at 16 days of depuration. The depuration half-life of the residues in the whole fish was not reported. The depuration rate constant (K_2) was not reported.

The lipid content of the fish was 3.5% at the start of the exposure (day 1) and increased to 6.4% at the end of depuration (day 16 of depuration; day 44 of study).

During exposure, one fish died in the high-dose group on day 5; this was considered not to be a substance-related effect. No changes in appearance and behavior were observed.

Study Acceptability: This study is classified as **supplemental/reliable with restrictions**. No significant deviations from good scientific practices were noted. The high-dose depuration data are unreliable. Fish tissue and water samples were not analyzed for [^{14}C]saflufenacil or its transformation products.

MATERIALS AND METHODS

Bluegill sunfish (*Lepomis macrochirus*; Osage Catfisheries, Inc., Osage Beach, Missouri) were acclimatized in glass aquaria (80 x 35 x 55 cm) at 23 ± 2°C, fed a diet of standard fish-feed (Ecostart 17, BioMar, Denmark) and frozen brine shrimp (artemia), and held under artificial light (16-hour light/8-hour dark photoperiod) for at least 14 days prior to test initiation (no medication was provided; fish hatched on June 12, 2006; Appendix 1, pp. 33-34; Table 9, p. 75). Mortality was <5% per week during the acclimation period, and only healthy fish were used. At the onset of the study, the fish had a mean body weight of 1.04 g (range 0.83-1.24 g) and a mean body length of 5 ± 2 cm. The organism loading at study initiation was 0.19 g fish/L/day based on a flow rate of 20.8 L/hour (p. 12).

Prior to study initiation, stock solutions were prepared (five portions into 10-mL vessels) using a flow-through system with [phenyl-U-^{14}C]-labeled N′-{2-chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide (saflufenacil; radiochemical purity 97.7%; chemical purity 93.7%; specific activity 5.05 MBq/mg; batch number 825-1302) mixed with unlabeled saflufenacil (purity 93.8%; batch number COD-000515; light beige solid; water solubility 0.21 g/100 mL at pH 7 and 20°C; log P_{ow} 4.47 in pH 4 buffer and 5.13 in pH 7 buffer) at a ratio of 1:10 (p. 11; Appendix 1, pp. 31-32, 36; Figure 2, p. 49; Figures 4-5, pp. 77-78). The mixed test substances were then dissolved in dilution water, resulting in a 10 mg/L nominal concentration of the stock solution. The pH of the stock solution was adjusted to 7.

Continuous flow-through aquatic exposure systems were prepared using three 100-L glass aquariums (80 x 35 x 55 cm; one control, two treated) with silicon rubber seals, provided with an overflow at *ca.* 36 cm, and maintained at 23 ± 1°C with a photoperiod of 16 hours light/8 hours dark (Appendix 1, p. 34). The test system was illuminated by fluorescent tubes positioned from the room ceiling. The dilution water was unchlorinated tap water obtained from the municipal water works mixed with deionized water, and adjusted to a hardness of 100 mg/L $CaCO_3$. The dilution water was saturated with oxygen; the aquaria were not aerated. [^{14}C]Saflufenacil was delivered to the mixing vessels using a pump (further details, including the flow rate, were not provided). The method used to supply the filtered, temperated dilution water to the mixing vessels was not reported. [^{14}C]Saflufenacil-treated dilution water was delivered into the treatment aquaria at a flow rate of 20.8 L/hour, at nominal dose levels of 1.0 µg/L and 10 µg/L (Appendix 1, p. 35).

The test aquaria were filled with non-aerated, dilution water that was saturated with oxygen (*ca.* 100 L; Appendix 1, p. 34). [^{14}C]Saflufenacil was added using a pump (flow rate not reported). Following a 5-day equilibration period, 90 fish were transferred to each test aquarium (p. 12; Appendix 1, pp. 35, 39). The fish were fed at a rate of 1-2% of mean body weight per day, generally in two applications per day. Measurements of pH and oxygen concentration were recorded twice weekly on days 0, 3, 6, 10, 13, 16, 21, 24, and 27 of exposure and days 31, 34, 38, 41, and 44 of depuration (Appendix 1, p. 41; Tables 1-2, p. 51). Total organic carbon (TOC) was measured weekly on days -1, 0, 6, 13, 21, and 27 of exposure and days 34 and 41 of

depuration (Appendix 1, Table 4, p. 53). Temperature measurements were recorded daily (Appendix 1, Table 3, p. 52). The daily temperature fluctuation was measured continuously in the control aquarium. Hardness and unwanted contaminants in water were measured at the beginning of the uptake period (day 0; Appendix 1, p. 34; Table 10, p. 76). The flow rates were monitored and the function of the metering pumps was checked daily.

During exposure, five fish were collected from each control, low-dose, and high-dose test vessel using a net, and were separated into filet (edible parts), head (non-edible parts), organs (non-edible parts), and carcass (non-edible parts) after 1, 2, 4, 7, 14, 21, 24, and 28 days of exposure (p. 13; Appendix 1, pp. 39-40, 42). Additional fish (10) were collected after 14 and 28 days of exposure for the identification and quantification of transformation products. Two control fish were used for blank correction, and the remaining three control fish were used for lipid analysis. The 16-day depuration phase was initiated by transferring the remaining fish from the control and exposure test vessels to fresh test vessels, continuously replenished with uncontaminated dilution water at the same nominal rate of 20.8 L/hour. Following depuration, five fish were collected after 1, 2, 4, 8, and 16 days from the treated and control aquaria, and were separated into filet (edible parts), head, organs, and carcass. Water samples were collected after 1 and 2 days of depuration from the exposed and control aquaria.

Water: Duplicate water samples (10 mL) were collected from the middle of the control and exposure test aquaria after -1, 0, 1, 2, 4, 7, 14, 21, 24, and 28 days of exposure and after 1 and 2 days of depuration (p. 13; Appendix 1, pp. 40, 42). Each sample was analyzed by LSC to determine the total radioactivity.

Additional water samples (1 x 1 L) were collected from the middle of the exposure test aquaria after 8, 14, and 28 days of exposure for the determination of transformation products (Appendix 1, pp. 37, 42). The samples were filled into glass flasks, which were saturated with the test solution from the test aquarium beforehand. The samples were not further analyzed.

Additional water samples were collected on unscheduled days (one sample/ day) in order to control the proper function of the dilution system (Appendix 1, p. 42). The samples were analyzed by LSC using a 1 minute counting program. The values obtained from the samples were of lower accuracy; therefore, these results were only used for adjustment of the dilution system.

Fish: During the exposure and depuration periods, five fish were randomly selected from each test vessel, sacrificed by a short incubation into a solution with a narcotic, and separated into fillet, head, organs, and carcass (p. 13; Appendix 1, pp. 37, 39, 42-43). The samples were transferred into an extractor hood and dried for *ca.* 1 day at room temperature. The samples were then combusted and the evolved $^{14}CO_2$ was trapped to measure total ^{14}C activity using LSC; combustion efficiency was not reported. If combustion could not be performed the same day, the samples were stored at room temperature in glass vials.

Ten additional fish were collected after 14 and 28 days of exposure for the identification and quantification of transformation products of saflufenacil (p. 13; Appendix 1, pp. 37, 39-40, 43). The fish were sacrificed, dissected, and the fillets and inedible parts from each group were pooled and packed into glass flasks. The samples were not further analyzed.

Three control fish were collected after 1, 2, 4, 7, 14, 21, 24, and 28 days of exposure and 1, 2, 4, 8, and 16 days of depuration to determine total lipid content (p. 13; Appendix 1, pp. 39-40, 43). The fish were sacrificed and the edible and inedible parts were pooled to form a single sample for each interval. The samples were stored in a deep freezer at *ca.* -20°C until the end of the depuration period. The sample was homogenized and then extracted once by shaking with chloroform (10 mL) and methanol (20 mL), followed by an additional extraction with chloroform (10 mL; Appendix 1, Attachment, p. 80). The homogenate was filtered and the samples were shaken following the addition of a 10% NaCl solution (30 mL). The lower phase was separated and dried using Na_2SO_4. The residual lipid fraction was weighed following filtration and evaporation of the solvent. The organic phase was evaporated to a constant weight.

RESULTS AND DISCUSSION

Water quality parameters were monitored and maintained throughout the study period (Appendix 1, p. 41). Throughout the study, the water temperature was maintained at 23 ± 2°C in all test aquaria (Appendix 1, p. 48). In the control aquaria, the water temperature was maintained at 24.1°C (range 23.4-24.9°C; Appendix 1, Table 3, p. 52). Dissolved oxygen concentrations exceeded 60% saturation and ranged from 7.0-8.6 mg/L, and pH values ranged from 7.5-7.8 (Appendix 1, Tables 1-2, p. 51). The total organic carbon ranged from 1.0-2.0 mg/L (Appendix 1, Table 4, p. 53). The light intensity was not reported. The test solution flow rate to the individual test aquaria was 20.8 L/hour; the dilution water flow rate to the mixing chambers was not reported (Appendix 1, pp. 34-35). Ninety randomly selected fish at study initiation had a body weight of 0.83-1.24 g and a mean body length of 5 ± 2 cm (Appendix 1, p. 33).

During the exposure phase, mean corrected measured [^{14}C]residue dosing values were 1.05 ± 0.037 µg/L (range 0.99-1.10 µg/L; 105% of target) and 11.3 ± 0.206 µg/L (range 10.8-11.6 µg/L; 113% of target) for the low- and high-dose solutions, respectively (p. 14; Appendix 1, pp. 45-46; Table 7, p. 55). In the control aquarium, concentrations of radioactivity were within the expected background range.

Water samples were not analyzed for [^{14}C]saflufenacil or its transformation products.

During the exposure phase: In the fish tissue samples, [^{14}C]saflufenacil residues reached steady state within 14 days of exposure, with mean whole body concentrations of 4.81 µg/kg and 4.39 µg/kg at nominal concentrations of 1.0 µg/L and 10 µg/L, respectively, according to the study author (p. 15; Table 1, p. 16; Appendix 1, pp. 45-46; Table 8, pp. 56-58, 65-67). For the **low-dose study**, maximum mean [^{14}C]saflufenacil residues were 4.81 µg/kg (exposure day 14) in whole fish, 0.35 µg/kg (exposure day 21) in edible tissue, and 6.09 µg/kg (exposure day 14) in

inedible tissue (Appendix 1, Table 8, pp. 56-64). The study author calculated a mean BCF value of 3.91 for whole fish (Table 2, p. 17; Reviewer's Comment 3). Reviewer-calculated maximum mean BCF values were 4.63 for whole fish (14 days exposure), 0.33 for edible tissue (21 days exposure), and 5.86 for inedible tissue (14 days exposure; Reviewer's Comment 2). In edible and inedible tissue samples, [^{14}C]saflufenacil residues ranged from 0-0.35 µg/kg and 4.91-5.89 µg/kg at 21-28 days, respectively. For the **high-dose study**, maximum mean [^{14}C]saflufenacil residues were 17.87 µg/kg in whole fish (exposure day 24), 23.68 µg/kg in inedible tissue (exposure day 24), and 0.35 µg/kg in edible tissue (exposure day 21; Appendix 1, Table 8, pp. 65-73). The study author calculated mean BCF values of 1.0 for whole fish. Reviewer-calculated maximum mean BCF values were 1.57 for whole fish (24 days exposure), 0.03 for edible tissue (21 days exposure), and 2.08 for inedible tissue (24 days exposure). In edible and inedible tissue samples, [^{14}C]saflufenacil residues ranged from 0.00-0.35 µg/kg and 6.30-23.68 µg/kg at 21-28 days, respectively. The uptake rate constant (K_1) and kinetic bioconcentration factor (BCF_K) for whole fish, were not reported. Tissue samples were not analyzed for [^{14}C]saflufenacil or its transformation products. During exposure, one fish died in the high-dose group on day 5; this was considered not to be a substance-related effect (Appendix 1, pp. 28, 48). No changes in appearance and behavior were observed.

Following 16 days of depuration: [^{14}C]Saflufenacil residues in the whole fish decreased by a mean of 70.5% in the low-dose study and increased by a mean of 2.3% (high dose) at 16 days of depuration (Table 1, p. 16; Appendix 1, pp. 45-46; Table 8, pp. 56-58, 65-67). The depuration half-life of the residues in the whole fish was not reported. Mean lipid content in the whole fish after 14 days of depuration was 6.4% (Appendix 1, p. 47). The depuration rate constant (K_2) was not reported.

Lipid analysis: The lipid content of the fish was 3.5% at the start of the exposure (day 1) and increased to 6.4% at the end of depuration (day 16 of depuration; day 44 of study; p. 15; Appendix 1, p. 47).

DEFICIENCIES/DEVIATIONS

1. Water samples were not analyzed for [^{14}C]saflufenacil or its transformation products. Saflufenacil may have degraded during the study due to the alkaline conditions in the water. Concentrations of the parent compound and degradates should be monitored during the study to confirm that degradation is not unreasonable.

2. Fish tissue samples were not analyzed for [^{14}C]saflufenacil or its transformation products.

3. The radioactivity level in the high-dose fish rapidly decreased at the beginning of depuration, and then increased to a level of 11.12 µg/kg in whole fish (p. 14; Appendix 1, p. 46). The study author stated that this increase could be due to uptake of fish excreta that still contained radioactive test substance from the uptake phase. The author added that this effect can be considered as specific behavior of fish under these circumstances, and is not relevant to the

conclusion on bioaccumulation. However, data were not provided to support this explanation. For example, whether radioactivity was incorporated into tissues was not investigated and references were not provided that indicate this behavior has been observed elsewhere. Therefore, the high-dose depuration data are unreliable. However, OECD Guideline 305 indicates that the depuration phase of a study is unnecessary when uptake has been insignificant (*e.g.*, BCF <10), which is the case here. Therefore, this deficiency is not critical.

REVIEWER'S COMMENTS

1. The study was conducted according to USEPA Subdivision N Guideline §165-4, USEPA Ecological Effects Test Guidelines OPPTS 850.1730: Fish BCF (1996), and OECD Guideline No. 305, Bioconcentration: Flow-through fish test (1996; p. 9; Appendix 1, p. 28). The study was conducted in compliance with the OECD Principles of Good Laboratory Practice, German Principles of GLP, and meets the USEPA FIFRA (40 CFR Part 160) and TSCA (Part 792) GLP Standards (pp. 3, 9; Appendix 1, pp. 20, 24). Signed and dated Data Confidentiality, GLP, Quality Assurance, and Certification of Authenticity statements were provided (pp. 2-5; Appendix 1, pp. 20, 23-24). A Signatures page was also provided (Appendix 1, p. 21).

2. The reviewer calculated the maximum bioconcentration factors for total radioactive residues in edible and inedible tissues and in whole fish using the following equation:

    a. maximum concentration of TRR in tissue (µg/kg) ÷
    b. average concentrations of TRR in the water through the relevant interval (µg/L).

3. The study author calculated steady-state bioconcentration factors based on total radioactive residues from the mean value of the combustion data from days 21-28 of exposure (p. 15). The calculations were based on the mean concentrations of the test item in water during the uptake phase.

4. The radiochemical purity of [^{14}C]saflufenacil was confirmed at the end of the uptake period via HPLC analysis under the following conditions (Appendix 1, p. 38): solvent acetonitrile:bidistilled water:formic acid (600:400:1, v:v:v), flow rate 0.8 mL/min., with UV (270 nm) and radioactive flow detection. The radiochemical purity was 97.7-100% (Appendix 1, Figure 3, p. 50).

5. The method used to deliver the dilution water to the mixing vessels was not reported. A diagram of the test flow-through system is presented in Figure 2 of the study report (Appendix 1, p. 49).

Attachment 1: Structure of Parent Compound

Saflufenacil [BAS 800 H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N′-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide. N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

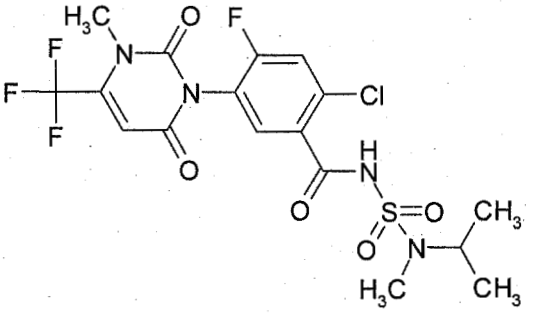
CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

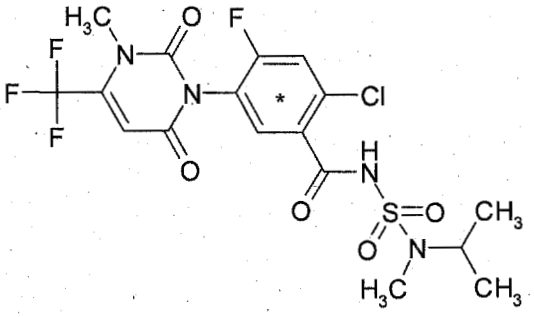
SMILES String: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

Empirical formula: $C_{17}H_{17}ClF_4N_4O_5S$ **Molecular formula:** $C_{17}H_{17}ClF_4N_4O_5S$

Unlabeled



[Phenyl-U-^{14}C]Saflufenacil



* = Location of the radiolabel.

Identified Compounds

Saflufenacil [BAS 800 H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N′-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide. N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

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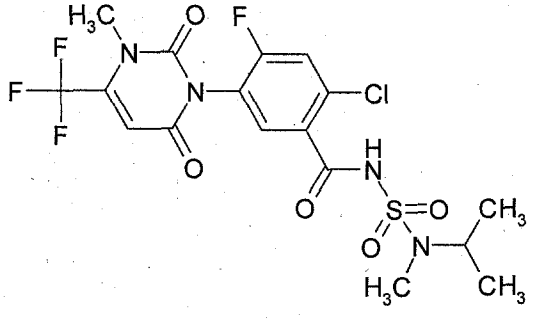
Empirical formula: $C_{17}H_{17}ClF_4N_4O_5S$ **Molecular formula:** $C_{17}H_{17}ClF_4N_4O_5S$



Attachment 2:
Illustration of Test System

Figure 2: Flow through system